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Monte Carlo(MC) simulation study on ammonia anchored TON zeolite for carbon dioxide capture SOOHO LEE, Sogang university, Nano-structured computer fluids lab — If zeolites are modified by ammonia, the electronic effect in ammonia resulted in different surface basicity of the zeolite materials. So, ammonia anchored materials show better adsorption rate of CO2 than pure materials at low pressure. MC simulations for CO2 adsorption were performed at 298K. The results show that, at pressure 1000 kpa CO2 loading is 1.404 mol/kg at ammonia anchored TON, and 0.529 mol/kg at pure TON. However, at high pressure, the ammonia effect becomes marginal. Ammonia anchored TON structures may be used to adsorb CO2 more effective than normal TON structure.

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